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PRODUCIBLE ALTERNATIVE TO CdTe FOR EPITAXY (PACE-2) OF LWIR HgCdTe

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1.0 INTRODUCTION AND OBJECTIVE

Described in the following report are the objective, approach, current results, and plans for the initial phase of the research program entitled, "Producible Alternative to CdTe for Epitaxy (PACE-2) of LWIR HgCdTe". Also described are alternate experimental avenues that were identified and added to the original proposed approach after initial experimental results from both this program and a preceding IR&D project. These additions will allow greater flexibility in the experimental approach toward achieving the program goal.

The long-term objective of this program is the demonstration of the feasibility of PACE-2 technology through fabrication and evaluation of multiplexed LWIR hybrid focal plane arrays fabricated in HgCdTe epitaxial layers grown on PACE-2 substrates. PACE is an acronym for Producible Alternative to CdTe for Epitaxy. Initially identified substrates for this program are Si and GaAs; both allow backside illumination in the LWIR region, are mechanically strong, and are available commercially as large, high purity wafers. The objective of the first phase of this program is to grow and analyze four layers each of LPE HgCdTe on CdTe/Si and CdTe/GaAs substrates in which the CdTe has been grown by vapor phase epitaxy (VPE).



2.0 APPROACH

Two distinct efforts are being pursued in order to achieve the objective of this program. First, the synthesis of a suitable alternate CdTe substrate and second, the growth of the active LWIR HgCdTe on that substrate.

2.1 Alternate CdTe Substrate Synthesis

Table 1 summarizes the growth techniques and base substrates that are being considered in the synthesis of the alternate CdTe substrate. The growth techniques selected for CdTe are Laser Assisted Deposition and Annealing (LADA), molecular beam epitaxy (MBE) and organo-metallic vapor phase epitaxy (OM-VPE) are all vapor phase deposition methods. The reason for selecting only vapor phase techniques in the growth on the selected base substrates is twofold. First, near equilibrium growth techniques such as LPE typically result in poor nucleation and subsequent poor growth for chemically dissimilar and lattice-mismatched systems such as considered here. Second, in this particular case, dissolution of the GaAs, Si or Ge would occur in the Te-rich liquid typically used for CdTe LPE.

We have added the OM-VPE to the two initially proposed vapor phase techniques, LADA and MBE in order to have the capability of growing CdTe at higher pressures and temperatures. Both the LADA and MBE techniques require a high to medium vacuum ambient which limits growth temperature to approximately 300°C due to the high vapor pressure of Cd. OM-VPE growth of CdTe can be carried out at atmospheric pressure in an inert gas ambient up to approximately 600°C.

Ge has been added as a base substrate to the originally proposed GaAs and Si substrate. Ge shares many of the advantages of Si and has, in addition, a more favorable thermal expansion match with CdTe.

To summarize the alternate CdTe substrate synthesis: three vapor growth techniques are used: LADA, MBE and OM-VPE; growth is carried out on three base substrates - GaAs, Si and Ge.



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Table 1
Growth Techniques and Base Substrates

Growth Technique	Characteristics			
	Pressure	Temperature	Growth Rate	In-Situ Analysis
LADA	low-med	0-400°C	1-10 $\mu\text{m}/\text{h}$	flux thickness monitor RGA visual
MBE	low	0-300°C	$\approx 1 \mu\text{m}/\text{h}$	flux RGA RED AES visual
OM-VPE	med-ambient	300-600°C	1-4 $\mu\text{m}/\text{h}$	visual

Base Substrates	Characteristics
GaAs	Polar, good thermal match
Si	Nonpolar, poor thermal match
Ge	Nonpolar, good thermal match

2.2 HgCdTe Growth

The LPE technique was chosen to grow the active HgCdTe layer because of its proven capability in producing device quality HgCdTe material. Growth is carried out in Te-rich liquids under a high pressure H_2 ambient in a graphite boat at approximately 500°C.



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Special precautions need to be taken with the alternate CdTe substrates, i.e., CdTe on GaAs, Si or Ge, in that the HgCdTe melt only contact the CdTe surface with which it is in near equilibrium. Melt contact of any part of the base substrate (GaAs, Si, Ge) results in dissolution of that substrate, with subsequent deleterious effects on the HgCdTe epitaxial layer, i.e., high dopant level or very poor epitaxy due to changes in the chemical composition of the melt. To reduce this risk, the LPE HgCdTe boat was modified with a special insert intended to allow contact of the HgCdTe melt to the CdTe surface only, and not the edge and backside of the base substrate.

In addition to the LPE technique, an isothermal vapor phase technique is also used to grow the active HgCdTe layers. Under development for the past two years on IR&D funds, it has shown the capability in producing device quality HgCdTe layers on both CdTe and PACE-1 (CdTe/sapphire) substrates. For example, in the past year device performance has been achieved with $R_0A > 10^7 \Omega\text{-cm}$ for $\lambda_c = 4.0$ at 77K and $R_0A > 2 \times 10^6 \Omega\text{-cm}$ for $\lambda_c = 4.65$ at 77K using bulk CdTe and PACE-1 substrates, respectively. This performance compares favorably with that found for LPE grown HgCdTe of the same composition.

A major attraction of the isothermal VPE technique is that it does not suffer from the liability of the LPE technique for PACE-2 applications - the chemical instability between base substrate and liquid.

The isothermal VPE technique has been used for PACE-2 growth on IR&D funds prior to the start of this program. The results will be described in Section 3.0.

To summarize, two techniques have been used to grow the HgCdTe layers. The baseline approach remains the LPE technique supplemented by an isothermal VPE technique.



3.0 RESULTS

This section describes progress in the synthesis of the alternate substrates and the growth of HgCdTe layers. For completeness and pertinence to this effort, results achieved on IR&D funds prior to the start of this program are also reported. Table 2 summarizes the progress to date.

Table 2
PACE-2 Growth Status Summary - CdTe and HgCdTe

Technique	Substrate		
	GaAs	Si	Ge
LADA	Good crystal by x-ray Good morphology Thick growth = 30 attempts	Semi-crystalline = 10 attempts	No attempts
	VPE HCT layers, n & p type LPE HCT chem. attack	VPE HCT - rough morphology (211)	
MBE	Good crystal by x-ray Good morphology Thick growth = 20 attempts	Good crystal by x-ray Nonuniform morphology Thin growth = 10 attempts	No attempts
	VPE/HCT layers, n-type LPE/HCT chem. attack	No VPE LPE/HCT slight chem. attack	
OM-VPE	Faceted morphology LPE improves morphology High dislocation density 3 attempts	Polycrystalline	Faceted morphology LPE improves morphology No character- ization ~ 10 attempts
	LPE/HCT chem. attack		LPE/HCT chem. attack 1 VPE n-type growth



3.1 LADA Growth of CdTe on GaAs and Si

LADA growth on GaAs is carried out in the following manner. GaAs substrates are oriented in the (100) direction to within $\pm 0.5^\circ$. Both n-type and semi-insulating substrates are used. The substrates are first degreased and etched, then placed on the substrate holder and the system pumped out. After the vacuum reaches mid 10^{-7} Torr, the GaAs substrates are flash heated to above 800°C for cleaning. Undoped CdTe is used as source. It is cleaned by scrubbing the surface with a focused laser beam. The substrate temperature at deposition is 350°C . The growth rate can be varied from $1 \mu\text{m}/\text{h}$ to $12 \mu\text{m}/\text{h}$ by increasing the laser power. The growth rate does not affect the layer quality based on results obtained so far. If the substrate surface is not treated uniformly, the grown layer is a mixture of rough and smooth regions. In early runs, the smooth region was less than 10% of the entire area. With optimization, the smooth region can routinely exceed more than 95% of the total area. Examples of a smooth layer is shown in Fig. 1, along with a Laue x-ray pattern, indicating (111) orientation for the CdTe deposit.

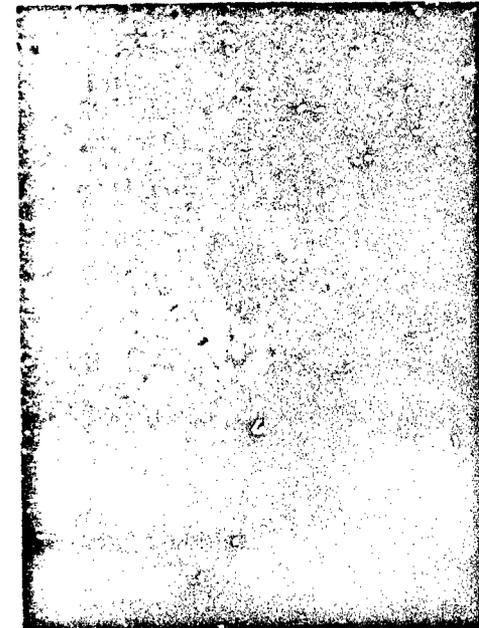
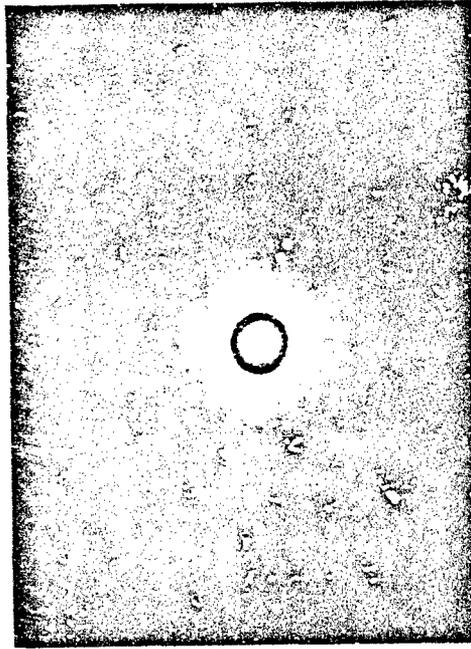
The quality of CdTe on GaAs has been examined by Transmission Electron Microscopy (TEM). Preliminary results indicate a transition zone of about $2 \mu\text{m}$ at the interface. This region has a very high density of misfit dislocation, as one would expect for a higher lattice mismatch system (Fig. 2). The density of dislocations decreases away from the CdTe/GaAs interface. At $6 \mu\text{m}$, it reached a plateau value of $\sim 10^4/\text{cm}^2$ which is as good as the best bulk CdTe material. LADA grown CdTe/GaAs layers have been used in several LPE and VPE HgCdTe growth.

LADA growth on Si of (111) and (211) orientations have not resulted in smooth looking layers, possibly due to remaining oxides. The current substrate heating capability is 800°C which is insufficient to efficiently remove all oxides from the Si surface.



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10 μm



X-RAY LAUE PATTERN

SURFACE MORPHOLOGY

Fig. 1 Morphology and x-ray Laue diffraction of a CdTe (111)/GaAs (100) layer.



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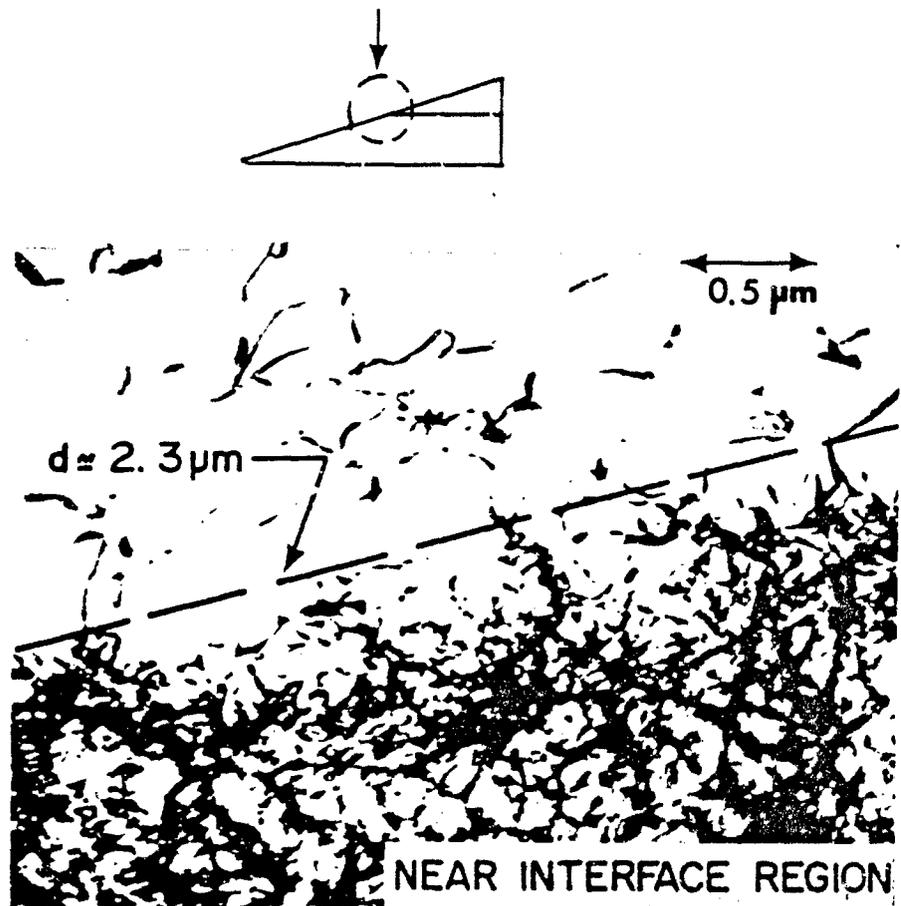


Fig. 2 LADA deposition - CdTe/GaAs (near interface region).



3.2 MBE Growth of CdTe on GaAs and Si

CdTe layers have been grown on (100) and (111)As terminated GaAs and (111) and (211)Si substrates. CdTe layers are grown using a flux of Cd and Te₂ derived from a heated graphite crucible filled with bulk CdTe. The starting CdTe material is obtained commercially, is of high purity, and is nominally undoped.

3.2.1 Substrate Preparation

The GaAs wafers are prepared by wet chemical etching to a procedure developed for previous III-V work. After heating to ~ 580°C, no carbon, oxygen or other impurities are detected by Auger electron spectroscopy (AES) and well developed (by reflection electron diffraction (RED)) (2 x 8) As stabilized surfaces are obtained for GaAs(100) and stepped (2 x 1) 60° patterns are observed on GaAs(111)As. The Si wafers are thoroughly cleaned in solvents and acids and given a final HF:H₂O (1:5) spin etch, rinsed with water and blown dry. AES of these as-prepared surfaces show no contaminants other than oxygen (< 1 monolayer), and no component of the Si (76 eV)/SiO₂ line is observed. Sharp (7 x 7) patterns for Si(111) can be obtained by heating to ~ 850-900°C. The Si(211) (2 x 2) pattern can also be obtained by the same procedure.

3.2.2 Nucleation of CdTe

The apparent sticking coefficients of Cd and Te onto the clean surfaces of all substrates investigated are functions of substrate temperature, coverage and incident flux level. For high temperatures (T > 600°C), neither Cd nor Te will bond to surfaces of GaAs or Si. For temperatures above a 'critical' temperature (T₁, a function of the particular substrate used and its orientation, usually near 300°C), exposure to CdTe beams for several hours will show only ~ 0.5 monolayers of Te bound to the surface and no Cd is detected (by AES). The RED pattern observed for these Te stabilized surfaces is the (1 x 1) bulk reconstruction for all substrates.



3.2.3 Nucleation onto GaAs

For $T < T_1$, where CdTe films accumulate, the RED patterns indicate that film growth is by island formation and coalescence, and superimposed GaAs(111) and film patterns are observed during nucleation. The (2 x 2) CdTe(111) reconstruction is observed immediately after nucleation and no 'healing' depth is required. Similar results are obtained on GaAs(100). If the substrate temperature is held below T_1 , single crystal CdTe films are obtained using a bulk CdTe source if the nucleating surfaces are clean. The growth rate is dependent upon the substrate temperature in that the net growth rate is determined by the impinging flux of Cd and Te_2 and the re-evaporation rate at that substrate temperature. The resulting surface morphology is smooth and cleaved edges observed by optical microscopy show no gross interfacial alloying (Fig. 3). CdTe growth on GaAs(111)As surfaces has resulted in CdTe(111)Te growth. In contrast, as also found for LADA CdTe/GaAs growth, either (111) or (100) orientations can be obtained using GaAs(100) substrates, depending upon the nominal surface reconstruction for GaAs(100) and the growth parameters. This phenomenon is reproducible, but is not understood at this time.

3.2.4 Nucleation onto Si

The keys to successful growth involve obtaining clean Si surfaces, nucleating a thin (< 10Å) layer of CdTe onto Si(111) at $T < T_1$, and then adjusting the substrate temperature so that the adsorption rate is slightly greater than the desorption rate so that the total growth rate is ~ 50-1000Å/h to provide a slow growth/annealing step. Extensive characterization indicates that single crystal CdTe with bulk-like properties can be obtained for films < 500Å thick on Si(111).

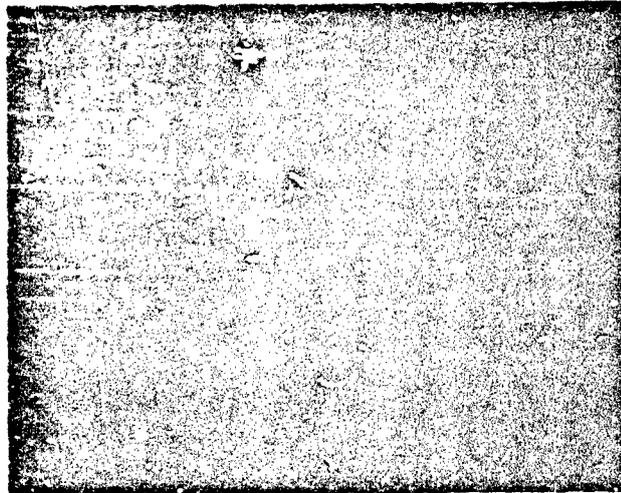
RED studies of CdTe grown onto (211)Si indicate that the nucleation process involves polycrystalline and amorphous growth of CdTe near the surface. Feature free layers have not been obtained. The x-ray rocking curve measurements, however, indicate that the crystal quality is adequate, further evidenced by successful CdTe LPE growth.



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30 μm

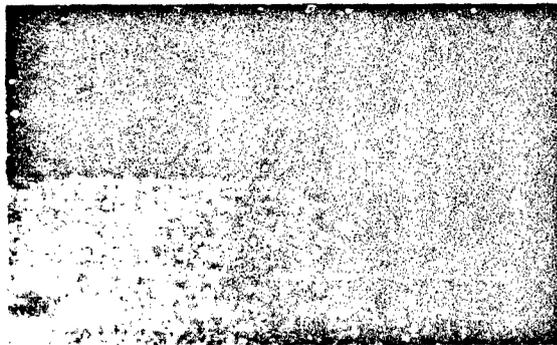


Fig. 3 MBE grown CdTe on GaAs. a) surface morphology; b) cross-section.



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The major drawback of MBE CdTe growth on Si is the time required for nucleation which must be operator assisted (via RED pattern observation) on a continuous basis up to ten hours. Attempts to accelerate the nucleation process thus far have led to inferior quality CdTe layers.

3.2.5 MBE CdTe Layer Characterization

Nomarski phase contrast microscopy has been used to observe the surface morphology and cleaved edges of films grown as thick as 25 μm . Feature free surfaces (cf. Fig. 3) are obtained on GaAs(111)As, GaAs(100) and Si(111) under proper growth conditions and surface preparation. Cleaved edge observations indicate no gross alloying at the substrate film interface, and SIMS studies show that at least the CdTe(111)/Si(111) interface is abrupt. AES measurements on grown surfaces show stoichiometric CdTe ratios for growth temperatures up to $\sim 300^\circ\text{C}$. UV reflectance data on all substrates provide spectra comparable to bulk grown CdTe.

An estimation of the relative crystalline perfection of the epitaxial layer is obtained from double crystal x-ray rocking curve measurements. The data are compared in terms of the full width at half maximum of the diffracted intensity as a function of angle. Table 3 lists comparative results on several substrates compared to measurements on bulk grown CdTe. Also included are results from layers on which an additional CdTe layer has been deposited by LPE.



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Table 3
X-Ray Rocking Curve Measurements for CdTe Grown on Various Substrates

Substrate	Thickness μm	Growth Rate $\mu\text{m}/\text{H}$	$\Delta\theta$ min	θ_{hkl}	$\Delta a/a^{(1)} \times 10^{-3}$
CdTe	bulk	---	1.8	(111)-11.9°	2.4
GaAs(100)	17.9	1.1	2.3	(100)-28.4°	1.2
GaAs(111)As	7.0	1.0	3.9	(111)-11.9°	5.4
Si(111)	.06	.005	3.3	(111)-11.9°	4.5
Si(111)	1.5	.06	5.3	(111)-11.9°	7.3
Si(211)	5.0	1.3	4.9	(211)-35.6°	1.9
Si(111)LPE ⁽²⁾	20	---	2.2	(111)-11.9°	3.0
Si(211)LPE ⁽²⁾	25	---	1.9	(211)-35.6°	.77

- (1) The quality $\Delta a/a$ ($= \Delta\theta \text{ ctn } \theta_{hkl}$) gives a measure of the distribution of lattice parameter in the layers.
(2) Additional CdTe deposited by LPE onto MBE grown CdTe.

A comparison of $\Delta a/a$ values indicates that the spread in lattice parameter (affected by low angle grain boundary formation, twinning, stoichiometry, etc.) for all samples measured is comparable to bulk values and, in the case of CdTe grown on GaAs(100) and Si(211), an improvement is observed. The minimum $\Delta a/a$ is observed for additional CdTe deposited by LPE onto CdTe grown onto Si(211) by MBE.

To summarize, MBE growth of CdTe onto GaAs and Si substrates of various orientations has been accomplished. CdTe growth of GaAs is fairly straightforward. Growth on Si substrates, however, is difficult due to a long nucleation process. RED, AES, UV reflection, laue and x-ray rocking curve measurements indicate bulk characteristics for CdTe layers grown on properly prepared surfaces and under optimum growth conditions. These layer also have virtually feature free surfaces, sharp interfaces and high IR transmission.



3.3 OM-VPE Growth of CdTe

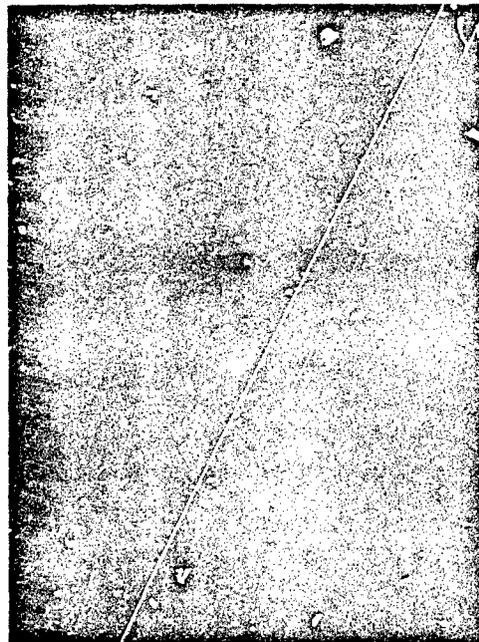
CdTe layers have been grown by OM-VPE on Ge and GaAs substrates of (111) and (100) orientations. The (111) layers on both substrates feature rough, strongly faceted morphologies that smooth out with a CdTe LPE layer overgrowth. Figure 4 shows the surface morphology of LPE CdTe grown on OM-VPE CdTe on a) GaAs and b) Ge. Growth on (111)As and (111)Ga terminated GaAs results in (111)Te and (111)Cd terminated CdTe, respectively. Growth on (100) surfaces is polycrystalline for both GaAs and Ge substrates.

Extensive characterization of these layers has not been carried out, most being used for trial HgCdTe LPE runs. Cathodoluminescence of LPE CdTe on OM-VPE CdTe/GaAs (Fig. 5) shows a defect structure similar to that found for PACE-1 CdTe. IR transmission (Fig. 5) shows high IR transmissivity and distinct interference fringes, indicating flat interfaces. (Absolute transmission is less than 100% since no antireflection coatings were used.)



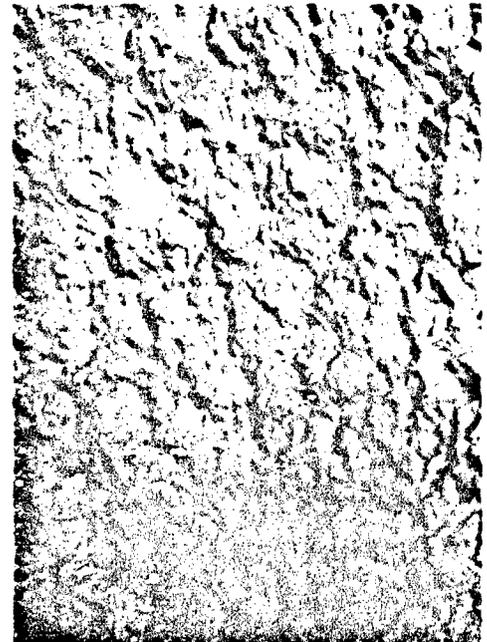
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(111)Te



GaAs SUBSTRATE

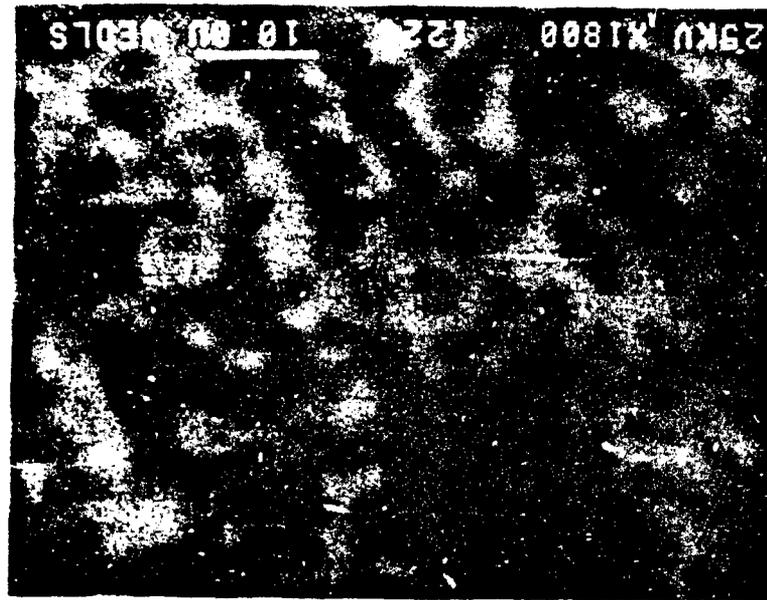
(111)Cd



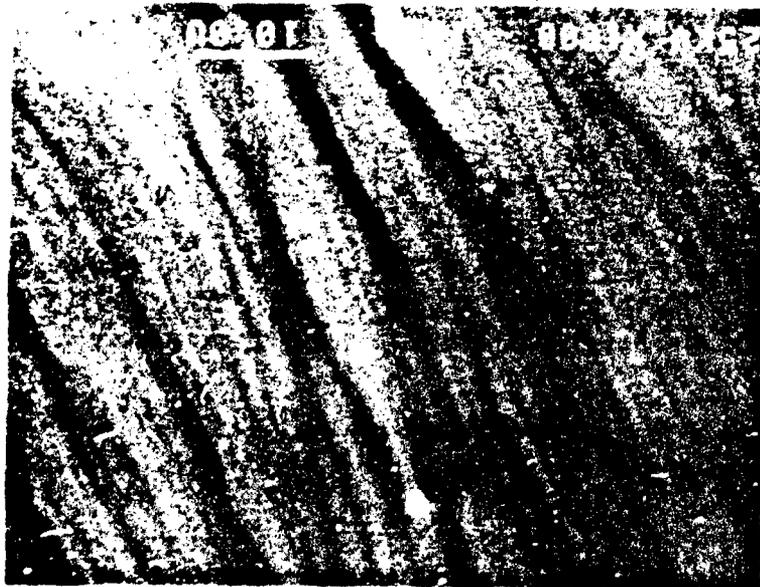
Ge SUBSTRATE

130 μm

Fig. 4 CdTe I.P.E on OM-VPE grown CdTe.



(b) CATHODOLUMINESCENCE IMAGE



(a) SURFACE MORPHOLOGY

Fig. 5 Cathodoluminescence of LPE CdTe on OM-VPE CdTe/GaAs.

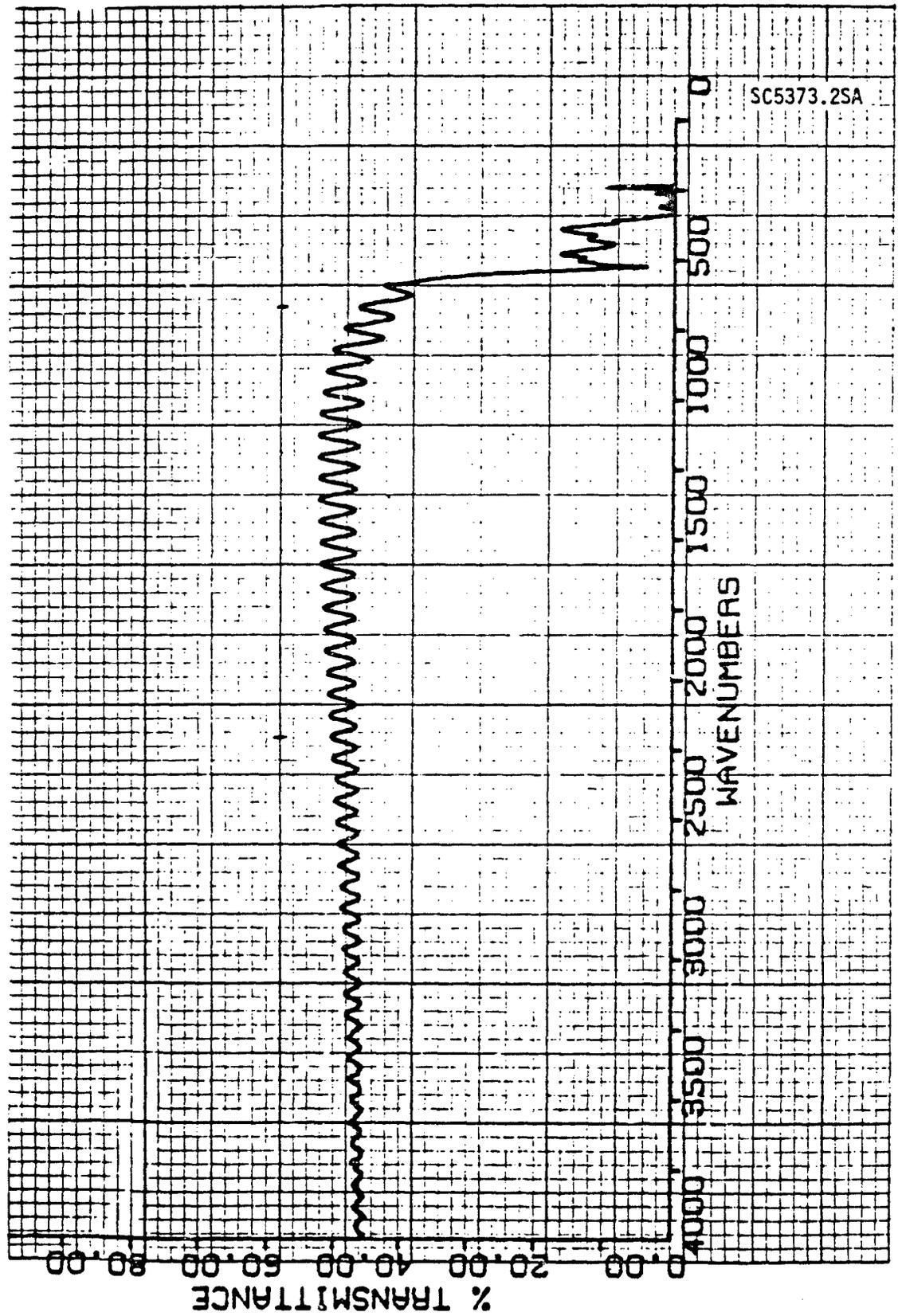


Fig. 6 IR transmission of LPE CdTe on OM-VPE CdTe/GaAs.



4.0 HgCdTe GROWTH ON CdTe/GaAs AND CdTe/Si SUBSTRATES

Reported in this section are the results obtained for HgCdTe growth, by LPE and isothermal VPE, on CdTe/GaAs and CdTe/Si substrates grown by LADA, MBE and OM-VPE techniques.

4.1 HgCdTe LPE Growth

A total of eleven LPE HgCdTe growths were attempted. Five attempts on CdTe/Ge substrates (OM-VPE), five on CdTe/GaAs substrates (2 MBE, 2 LADA, 1 OM-VPE), and one on a CdTe/Si substrate (MBE).

Precaution was taken to confine the HgCdTe melt to the central portion of the substrate and away from the edges where chemical attack of the base substrate could occur. Despite these precautions, partial dissolution of the base substrate occurred in each case due to chemical attack by the LPE melt. Figure 7 shows the front or epi-side, as well as the backside of LPE HgCdTe growth attempt 2-732 on a MBE grown CdTe/GaAs substrate. Chemical attack of the GaAs substrate occurred in two modes. In one mode, the melt attacked the substrate at one edge, as can be seen in the upper right hand corner of the backside photo. The other mode of chemical attack occurred through the CdTe layer itself via regions of poor crystallinity that allowed the melt to communicate with the GaAs substrate, leading to chemical dissolution that is visible as spots on the backside of the GaAs wafer. Shown in Fig. 8 are details of the surface morphology and cross-section of the HgCdTe/CdTe/GaAs layer. The surface morphology is fairly rough and partly due to the contamination of the melt by the partial chemical dissolution of the GaAs substrate. The cross-section of the wafer, obtained optically from a section of the wafer, shows clearly the top HgCdTe layer, the CdTe layer and the GaAs substrate. IR transmission (Fig. 9) indicated HgCdTe material in the MWIR range with low transmission due to both the rough surface and a highly doped layer because of the contaminated melt. Hall and SIMS analysis were not carried out, since high doping levels were expected due to the chemical attack of the GaAs substrate.



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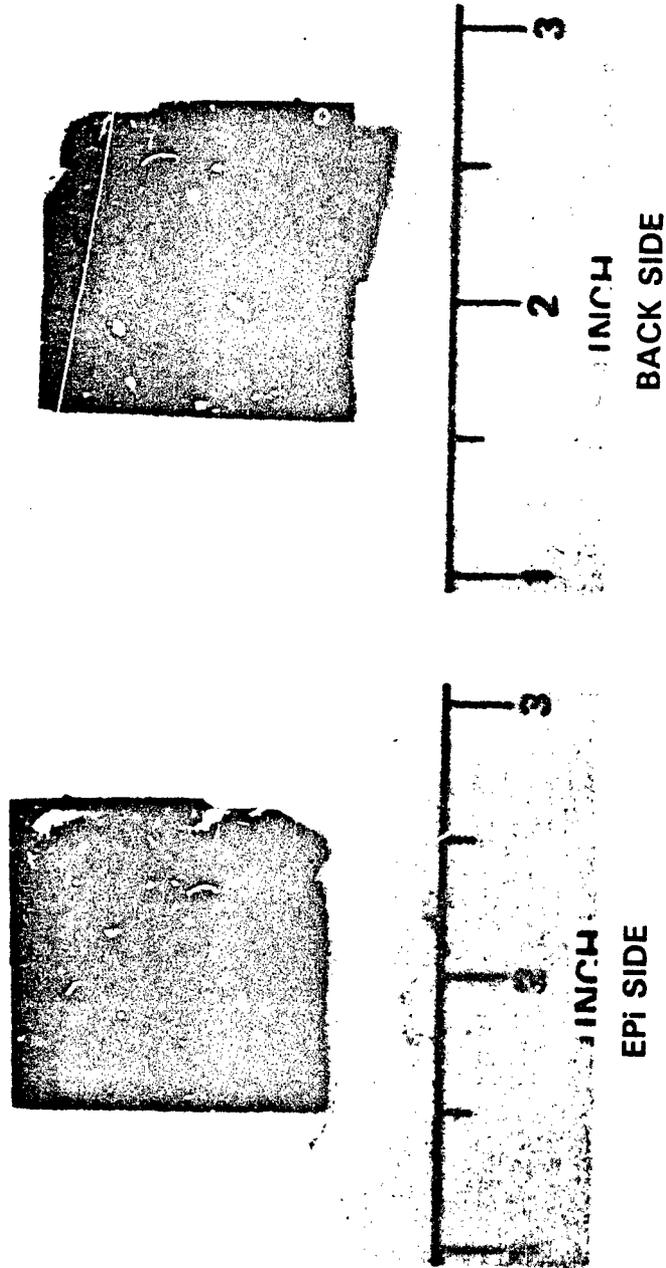
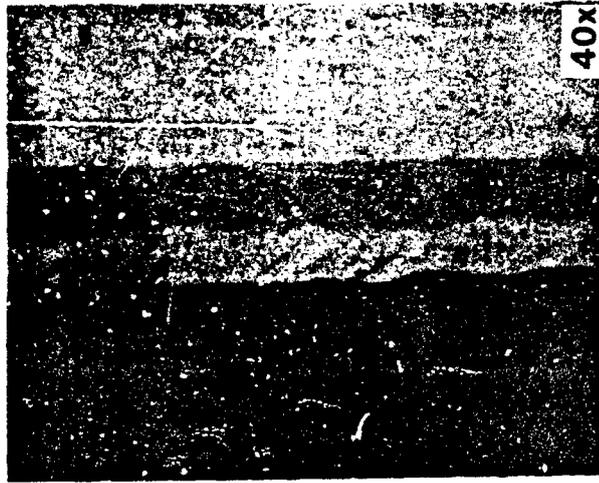


Fig. 7 Photograph of HgCdTe LPE growth on MBE CdTe/GaAs substrate.



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CROSS-SECTION



SURFACE MORPHOLOGY

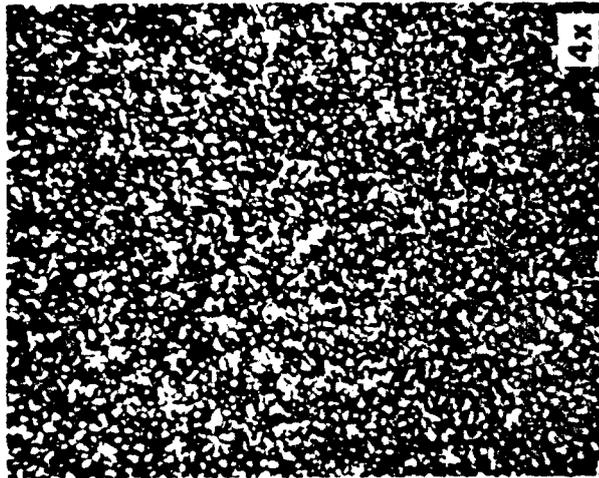


Fig. 8 HgCdTe LPE growth on MBE CdTe/GaAs substrate.



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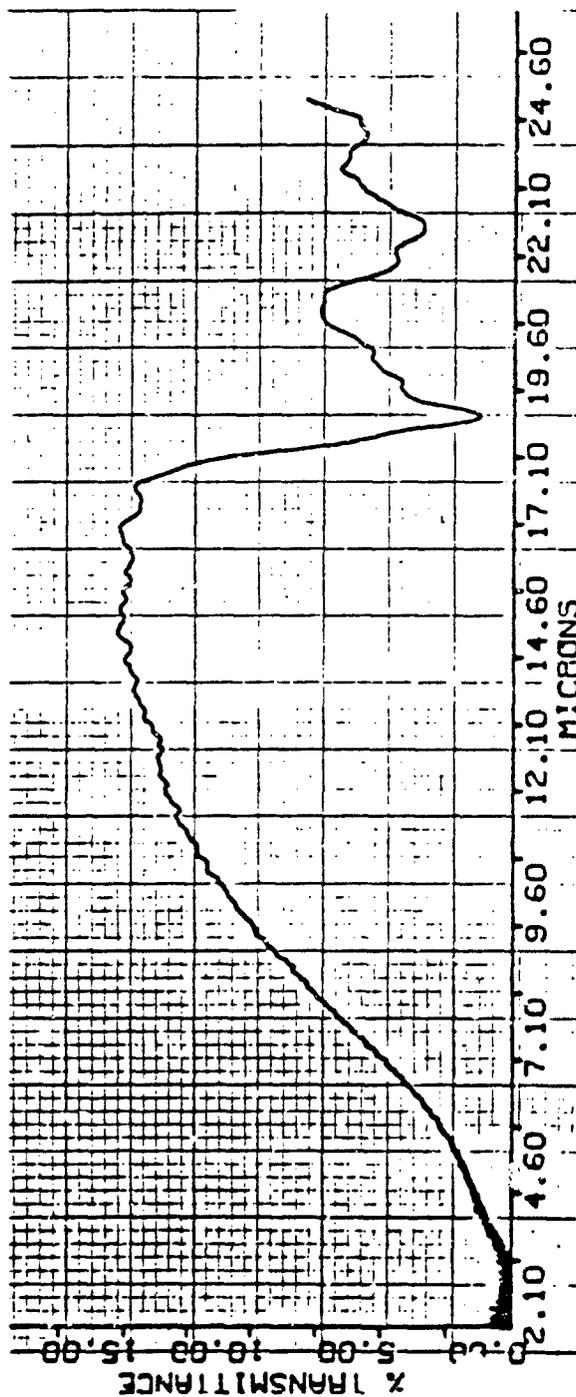


Fig. 9 IR transmission of LPE HgCdTe on MBE CdTe/GaAs substrate.



Similar results were obtained for CdTe/Ge and CdTe/Si substrates, although the Si base substrate suffered the least amount of chemical attack.

4.2 Isothermal VPE Growth of HgCdTe

Use of this growth technique resulted in epitaxial HgCdTe layers on several PACE-2 CdTe substrates. Chemical attack of the base substrate does not occur with this growth technique. Properties of VPE grown HgCdTe layers on PACE-2 substrates are summarized in Table 4. Also included is data for layers grown on PACE-1 (CdTe/sapphire) and bulk CdTe substrates. Following is a more detailed description for VPE growth on various PACE-2 substrates.

Except for two layers (1344 and 1414), all VPE grown HgCdTe layers on PACE-2 substrates have had n-type conduction in contrast to the p-type conduction routinely obtained on bulk CdTe and PACE-1. The mechanism causing the n-type conduction in PACE-2 growth is currently being studied by Hall and SIMS analysis.

4.2.1 VPE HgCdTe Growth on LADA CdTe/GaAs

The substrates were LADA grown CdTe layers on (100) GaAs substrates. The surface of the grown VPE HgCdTe layer was optically mirror smooth. Figure 10 shows micrographs of the cleaved cross-section and of the surface morphology. Laue x-ray analysis showed its orientation to be (100). Carrier concentrations and mobilities were measured by the Van der Pauw technique and are summarized in Table 4. VPE HgCdTe growth was also tried on a LADA (211) CdTe/Si substrate. The surface morphology of both the (211) CdTe/Si substrate and the VPE HgCdTe layer on that substrate were not as smooth as those found for CdTe/GaAs substrates and are shown in Fig. 11.

4.2.2 HgCdTe VPE Growth on MBE CdTe/GaAs Substrate

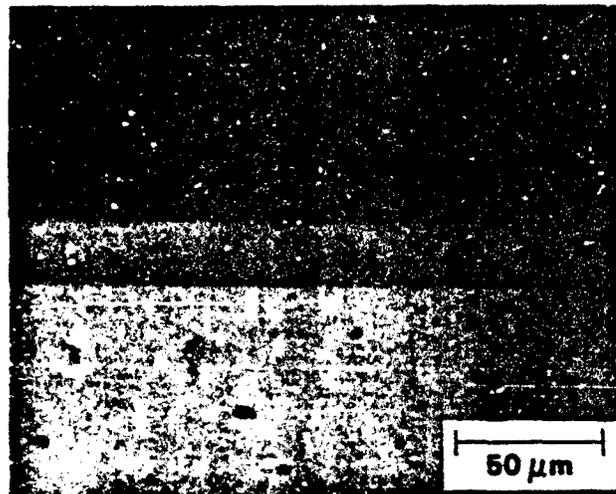
MBE grown CdTe on GaAs were used as substrates for the VPE growth of HgCdTe. Results obtained for VPE HgCdTe growth on MBE CdTe/GaAs are similar to those for LADA CdTe/GaAs substrates, described in Section 4.2.1. Carrier



Table 4

VPE Growth No.	Substrate	Orienta- tion and Polarity (CdTe)(Substrate)	Thickness (μm)	Type	Wavelength (300K) μm	Resistivity $\Omega\text{-cm}$	Carrier Mobility ($\text{cm}^2/\text{V-s}$) 77K	Concentration cm^{-3} 77K
1341	Bridgman CdTe	(111)Te	25	P, Hg-anneal	6.25	0.48 0.43	359 576	3.5×10^{16} 2.5×10^{16}
1373	Bridgman CdTe	(111)Te	15	P	3.03	0.35	234	8.7×10^{15}
1374	Bridgman CdTe	(111)Te	12	P	2.87	0.33	321	6.7×10^{15}
1344	LADA CdTe/GaAs	(100)	16	P	6.0	0.22	169	1.7×10^{17}
1387	LADA CdTe/GaAs	(111)Te/(100)	7	n	6.3	5.3×10^{-3}	5.7×10^3	2×10^{17}
1388	LADA CdTe/GaAs	(100)	10	n	6.0	2.4×10^{-3}	1.3×10^4	1.9×10^{17}
1414	LADA CdTe/GaAs	(111)Te/(100)	6	P	4.5		155	2.4×10^{16}
1378	LPE PACE-1 CdTe	(111)Cd	22	P	3.88	0.31	306	5.2×10^{15}
2343	OM-VPE PACE-1 CdTe	(111)Te	20	n	6.0	0.147 0.40	1.3×10^4 366	3×10^{14} 4.2×10^{16}
1401	OM-VPE CdTe/Ge	(111)Cd	6	n	6.0	9.0×10^{-3}	1.1×10^4	5.7×10^{16}
1377	MBE CdTe/GaAs	(111)Te(100)	4	n	6.0	2.6×10^{-2}	1.1×10^4	2.1×10^{16}
1400	MBE CdTe/GaAs	(111)Te(100)	11	n	6.0	9.0×10^{-3}	1.1×10^4	5.8×10^{16}

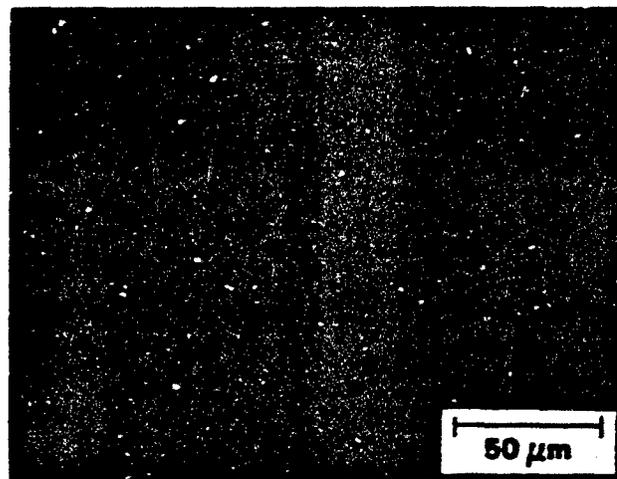
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HgCdTe (100)
CdTe (100)

GaAs (100)

(a)

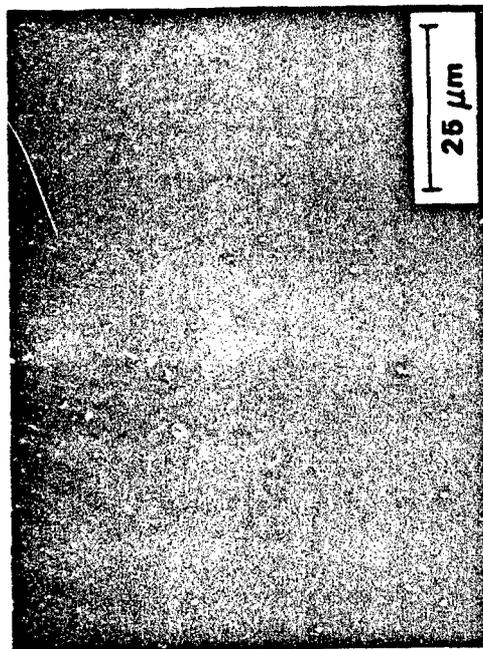


(b)

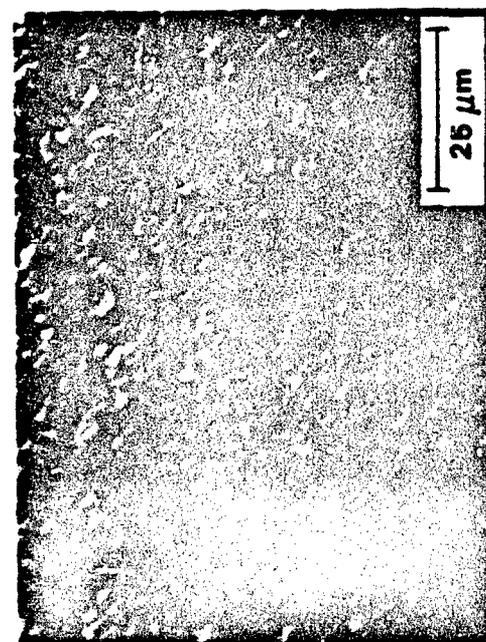
Fig. 10 VPE HgCdTe on a LADA CdTe/GaAs substrate. a) cross-section, b) surface morphology.



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(a)



(b)

Fig. 11 VPE HgCdTe epilayer grown on LADA CdTe/Si.



type, concentration and mobility for VPE HgCdTe on MBE CdTe/GaAs are tabulated in Table 4. SIMS analysis has been carried out to characterize the distribution of some impurities, base substrate elements, Ga and As in the epitaxial layer. Shown in Fig. 12 is the SIMS depth profile of an MBE grown CdTe on GaAs. The Ga level is constant and relatively high level with some structure prior to the interface. The As level is very low in the CdTe. Indium is also present at relatively high levels. Figure 13 shows the SIMS profile after HgCdTe VPE layer growth on an MBE CdTe/GaAs substrate. The impurity distribution has become complex showing impurity (Na and Li) and Ga spikes at the point of the original CdTe surface (part of the CdTe layer is consumed during isothermal VPE), and a sharp dropoff in impurity and Ga level toward the surface (last to grow HgCdTe). The As level remains low. Further analysis is needed to fully understand the behavior of the impurity distribution and out-diffusion of Ga from the GaAs substrate.

4.2.3 HgCdTe VPE Growth on OM-VPE CdTe/Ge

OM-VPE layers of (111)Cd terminated CdTe on Ge were used as substrates for HgCdTe VPE. Grown VPE HgCdTe layers had wavy surfaces due, in part, to the structured surface of the OM-VPE grown CdTe on Ge. The HgCdTe was also n-type, as shown in Table 4. Analysis is currently underway to determine the underlying reason for the n-type conduction mechanism. Surface morphology and the cross-sections of such a layer is shown in Fig. 14. The IR absorption spectrum is shown in Fig. 15.

4.2.4 Summary HgCdTe PACE-2 Growth

LPE and VPE growth have been carried out on several PACE-2 substrates grown by LADA, MBE and OM-VPE. In all LPE growth attempts, chemical attack of the base substrate (GaAs, Si, Ge) occurred, resulting in poor epitaxy due to chemical changes in the melt.

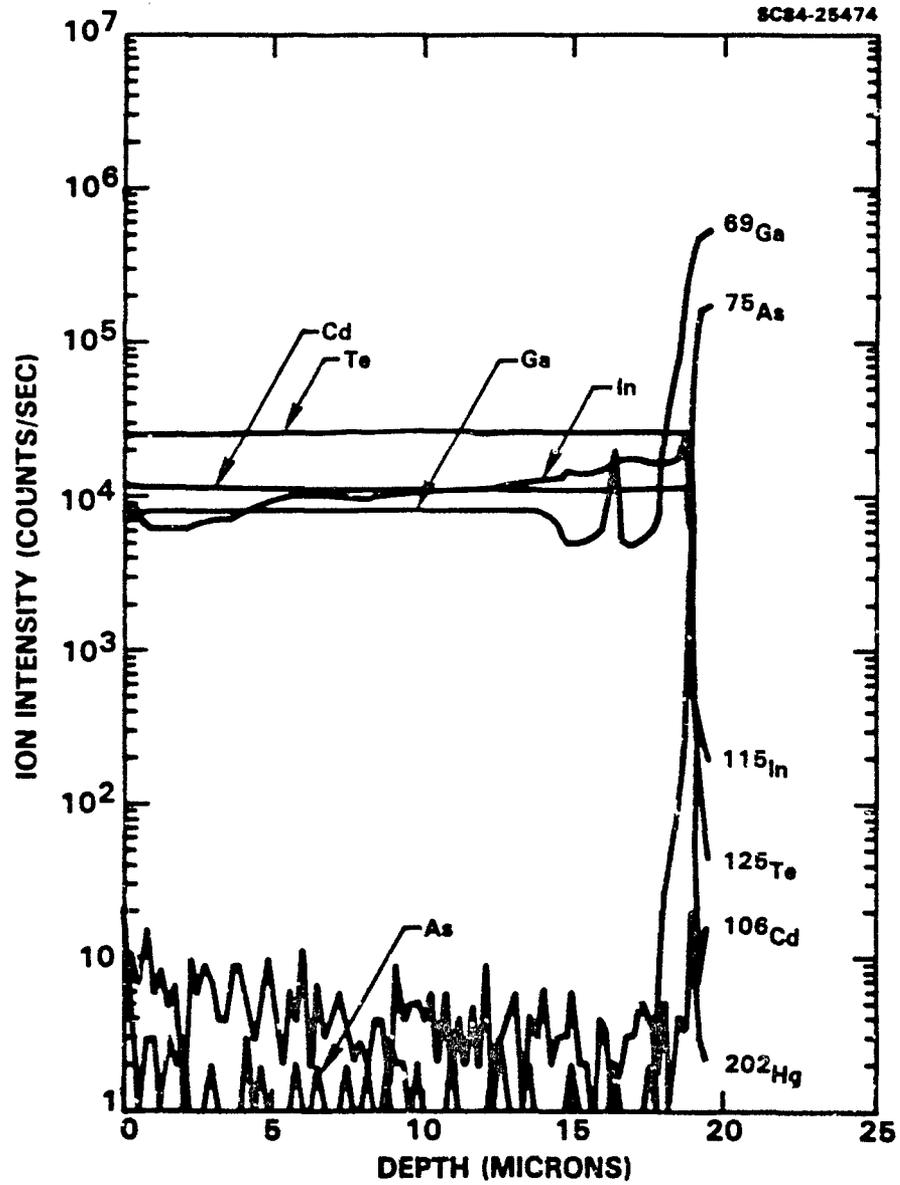


Fig. 12 SIMS depth profile of MBE CdTe/GaAs.

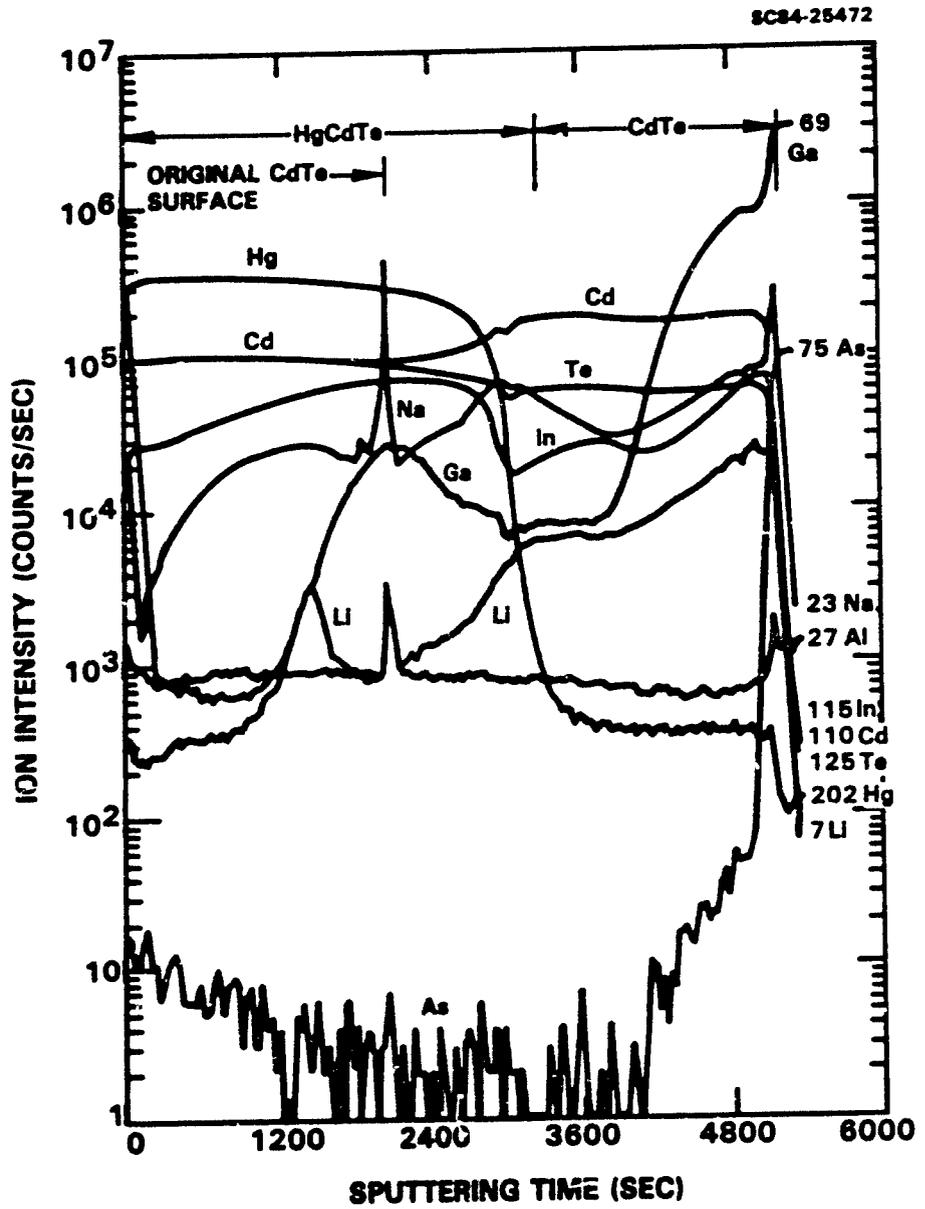
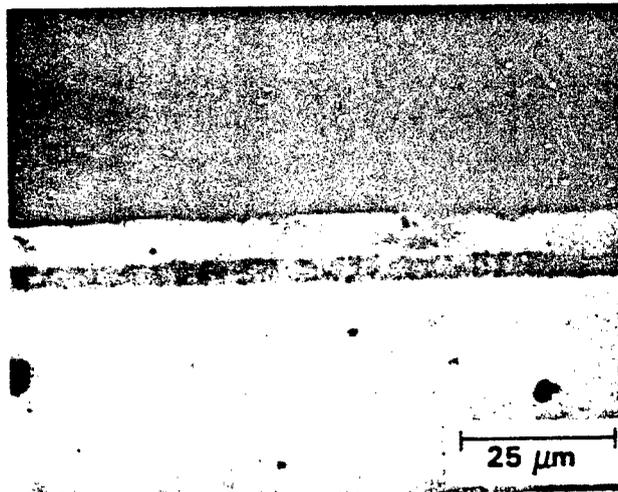


Fig. 13 SIMS depth profile of VPE HgCdTe on MBE CdTe/GaAs.



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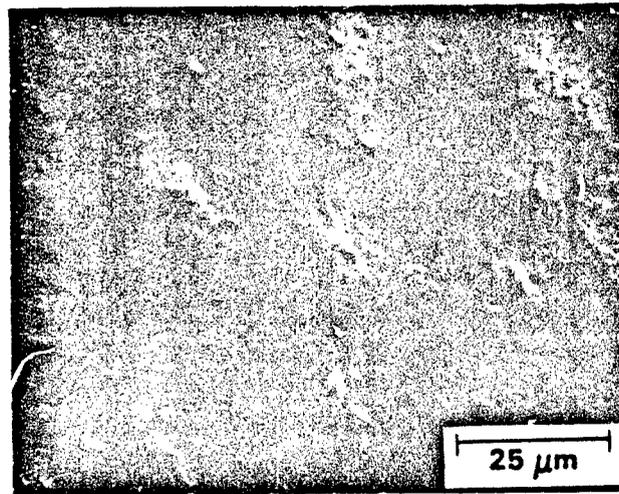


(VPE) HgCdTe

(OM VPE) CdTe

Ge (111)

a)



b)

Fig. 14 VPE HgCdTe layer on OM-VPE CdTe/Ge.

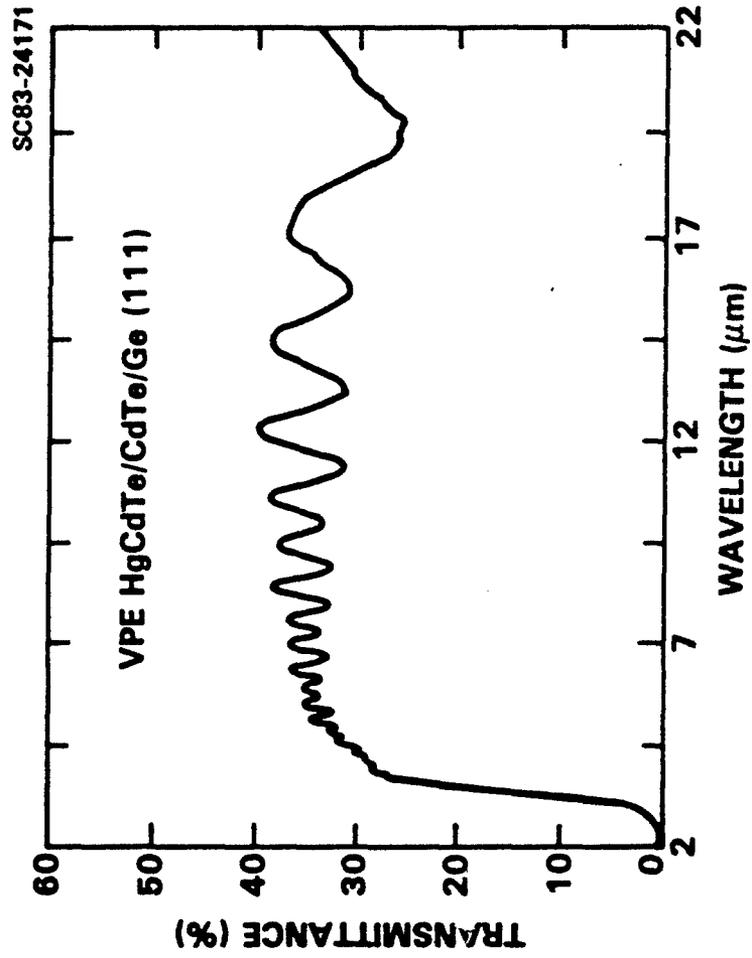


Fig. 15 IR transmission spectrum (300K) of VPE HgCdTe on CdTe/Ge.



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Epitaxial layers of HgCdTe were grown on FACE-2 substrates by the isothermal VPE technique. Grown layers were characterized for surface morphology composition, thickness, carrier type, concentration and mobility. Most layers had n-type conduction, possibly due to Ga outdiffusion for the case of GaAs substrates. SIMS analysis was carried out on selected samples. HgCdTe VPE layers grown on CdTe/GaAs substrates showed a complex depth distribution of impurities and Ga.



5.0 PLANS

Table 5 summarizes the plans for PACE-2 CdTe and HgCdTe growth activities.

For GaAs substrates, all three vapor phase techniques will continue to be pursued. Main emphasis, however, will be concentrated on the LADA and OM-VPE techniques. The rationale for this choice is that the quality of LADA and MBE grown CdTe on GaAs appear to be identical. LADA growth, however, is easier to carry out. OM-VPE growth of CdTe on GaAs will provide material grown at higher temperatures (comparable to subsequent HgCdTe LPE or VPE cycles) and is also capable of growing on large areas (2 in. diameter). Optimization will include refinement of the crystal growth parameters, establishing the best surface preparation and selecting the best orientation. OM-VPE CdTe/GaAs layers will be analyzed for carrier type, conductivity and crystallinity, since growth can be carried out $\approx 200^\circ\text{C}$ higher than for the MBE or LADA techniques. This may help improve the crystallinity of the CdTe layer; however, outdiffusion of Ga and As may also increase.

In the LPE HgCdTe growth on CdTe/GaAs substrates, the LPE boat will be further modified to provide greater physical separation between melt and the wafer edge to further reduce the risk of physical communication between base substrate and melt.

In addition, growth from supercooled melts will be attempted. This type of growth results in a very high initial growth rate and may prevent the "punch through" observed in all previous LPE growth attempts on CdTe/GaAs.

Once HgCdTe layers can be grown by LPE without obvious chemical contamination from the base substrate, Hall and SIMS analysis of the growth layer will be initiated to determine the outdiffusion of the base substrate elements in the CdTe and HgCdTe at the higher LPE growth temperatures (500°C vs 300°C for MBE and LADA).



Table 5
PACE-2 Plans

Technique	Substrate		
	GaAs	Si	Ge
LADA/ CdTe	Continue optimization Refine crystal growth parameters Optimize surface prep Use best orientation	Need AES & RHEED capability to properly prepare surface Small effort	No effort
MBE/ CdTe	Same Small effort	Explore the use intermediate layer to ease nucleation difficulties on Si in order to achieve uniformity.	Small effort
OM-VPE/ CdTe	Optimize growth param- eters and surface (large area, poten- tially higher crystallinity be- cause higher growth temperature)	No attempts (cannot prepare surface properly)	Optimize growth conditions and surface prepara- tion. Grow on high resistivity Ge substrates
LPE/ HgCdTe	Redesign graphite boat to revent chemical attack Use supercooled solution for fast initial growth Use Hall and SIMS characterization to establish outdiffusion of Ga and As	Attempt based on GaAs result	Attempt based on GaAs result
VPE/ HgCdTe	Establish growth con- dition for p-type growth Characterize with Hall and SIMS	Same as for GaAs	Same as for GaAs



Isothermal VPE will continue to be carried out on CdTe/GaAs to establish growth conditions for p-type HgCdTe layers. Planned experiments include faster growth rates and lower temperature growth. Grown layers will be analyzed with Hall and SIMS techniques.

For CdTe growth on Si substrates, we will use MBE only, since currently it is the only growth method with both the capability to properly prepare and analyze in situ the Si surface and subsequent growth. The use of thin, MBE evaporated, Ge buffer layers on Si will be explored as a way of alleviating the nucleation difficulties of CdTe on Si.

HgCdTe LPE growth on CdTe/Si substrates will be attempted if the LPE growth on GaAs substrates are successful. HgCdTe VPE growth will be carried out and analyzed for crystalline quality and background impurity concentration.

The main emphasis for CdTe growth on Ge substrates will be the OM-VPE technique. Some growth attempts will be made by MBE mainly as a control to the CdTe growth on Ge/Si.

For the OM-VPE growth on Ge, further optimization of the growth parameter is needed to improve the CdTe material quality. Again, HgCdTe LPE growth will only be attempted if successful on GaAs substrates. HgCdTe VPE growth on CdTe/Ge substrates will continue to be pursued along with material characterization.



6.0 SUMMARY

Uniform epitaxial layers of CdTe have been grown on GaAs, Si and Ge substrates by LADA, MBE and OM-VPE techniques. Bulk-like CdTe qualities have been measured for LADA and MBE grown CdTe on GaAs by TEM, x-ray diffraction and cathodoluminescence analysis. Single crystal growth of CdTe on (111) and (211) Si have also been achieved by MBE. Layers of CdTe on Si lack spatial uniformity because of an extended and difficult nucleation cycle. Improvement in crystallinity and a reduction in defect density has been found for CdTe layers grown by LPE on MBE CdTe/GaAs and CdTe/Si substrates. At this time, the quality of OM-VPE grown CdTe on GaAs and Ge substrates is inferior to that grown by MBE or LADA.

HgCdTe LPE growths on CdTe/GaAs, CdTe/Si and CdTe/Ge substrates resulted in chemical attack of the base substrate. HgCdTe growth by isothermal VPE on the same substrates have resulted in epitaxial layers of HgCdTe. Except for two cases on GaAs substrates, the layers had n-type conduction.

The remainder of this phase of the program will be structured in the following manner. CdTe growth on GaAs will be carried out by LADA to supply substrates for the HgCdTe LPE and VPE effort. LADA has shown itself to be the best technique from a quality/effort criteria for CdTe growth on GaAs. The MBE effort will concentrate on Si substrates. This technique has shown that high quality CdTe can be grown on Si. The use of intermediate Ge buffer layers on Si will be evaluated in easing the nucleation difficulties of CdTe directly on Si. OM-VPE growth of CdTe/GaAs will concentrate on Ge substrates where some success has been achieved.

CdTe/Si and CdTe/Ge substrates will be used in both HgCdTe LPE and VPE growth attempts. Grown HgCdTe layers will be analyzed for carrier type, concentration and mobility. X-ray diffraction and cathodoluminescence will be used to determine crystallographic quality and defect structure, respectively. SIMS will be used to determine the depth (distribution) of impurities and base substrate elements in the epilayers.



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At the conclusion of this phase of the program, we will use the information obtained in the above outlined effort to define a baseline PACE-2 approach. This will entail selecting a primary base substrate and a growth technique each for CdTe and HgCdTe. A backup PACE-2 approach will also be defined.